

Scattering lengths of calcium and barium isotopes

U. Dammalapati and L. Willmann*

*Kernfysisch Versneller Instituut (KVI), University of Groningen,
Zernikelaan 25, 9747 AA Groningen, The Netherlands.*

S. Knoop†

LaserLaB Vrije Universiteit, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands.

(Dated: October 26, 2011)

We have calculated the s -wave scattering length of all the even isotopes of calcium (Ca) and barium (Ba), in order to investigate the prospect of Bose-Einstein condensation (BEC). For Ca we have used an accurate molecular potential based on detailed spectroscopic data. Our calculations show that Ca does not provide other isotopes alternative to the recently Bose condensed ^{40}Ca that suffers strong losses because of a very large scattering length. For Ba we show by using a model potential that the even isotopes cover a broad range of scattering lengths, opening the possibility of BEC for at least one of the isotopes.

PACS numbers: 34.20.-b, 34.50.Cx, 67.85.-d

I. INTRODUCTION

Knowledge of the s -wave scattering length plays a crucial role in the achievement of Bose-Einstein condensation (BEC) in ultracold atomic gases [1]. A positive sign of the scattering length indicates that a Bose-Einstein condensate is stable whereas a negative sign indicates an unstable or collapsing condensate. Also its magnitude is crucial in the formation of BEC, as it determines the elastic and inelastic collision rates. For efficient evaporative cooling a large scattering length is required, however for a too large scattering length three-body recombination loss limits the formation and collisional stability of a BEC. This gives rise to a range of about $50 - 200a_0$ ($a_0=0.5292$ nm) that can be considered favorable.

Alkaline-earth elements and the alike ytterbium (Yb) system have been the center of attraction in ultra-cold atom research because of their unique atomic structure and the availability of different stable isotopes with zero nuclear spin (bosons) and with large nuclear spin (fermions). They are being used in frequency metrology [2–4] and are proposed for quantum information processing [5]. Recently, BEC has been achieved in ^{40}Ca [6], ^{84}Sr [7, 8], ^{86}Sr [9] and ^{88}Sr [10]. Also BEC of different Yb isotopes has been reported: ^{174}Yb [11], ^{170}Yb [12], ^{176}Yb [13] and ^{168}Yb [14], of which the last one has an abundance of only 0.13%, highlighting the possibility of using rare isotopes to achieve BEC.

In general, isotopes of an element have different scattering lengths. Therefore the ability of BEC formation depends crucially on the chosen isotope. For instance, the scattering length of ^{84}Sr is $123a_0$ [15], which made it an ideal candidate to achieve BEC despite its low abundance of only 0.6% [16], as compared to the more abun-

dant ^{86}Sr (10%, $800a_0$ [15]) and ^{88}Sr (83%, $-2a_0$ [15]), either suffering strong losses [9] or requiring sympathetic cooling with another isotope [10], respectively. The ^{40}Ca isotope has a large scattering length of about $440a_0$ [6], limiting the size and stability of BEC.

Motivated by the success of BEC in Sr and Yb even isotopes, and ^{40}Ca , we carried out calculations to obtain the scattering lengths for all the even (bosonic) isotopes of Ca and Ba, for which mass and abundance are summarized in Table I. Laser cooling and trapping of all stable Ca isotopes have been reported [17, 18]. The demonstration of magneto-optical trapping of Ba [19] has opened its use for ultra-cold collision studies, photoassociation spectroscopy and Bose-Einstein condensation. Recently, an optical clock based on ultracold Ba has been proposed [20].

II. THEORY

The scattering properties of ground state atoms are obtained from the underlying two-body ground state potentials. For alkaline-earth atoms there is only one molecular ground state potential, namely the singlet $X^1\Sigma_g^+$ potential. Furthermore, the lack nuclear spin and therefore hyperfine structure for the even (bosonic) isotopes highly

TABLE I: Mass and abundance of all stable even isotopes of Ca and Ba [21].

Calcium					
Isotope	40	42	44	46	48
Mass (amu)	39.963	41.959	43.955	45.954	47.953
Abundance (%)	96.941	0.647	2.086	0.004	0.187
Barium					
Isotope	130	132	134	136	138
Mass (amu)	129.906	131.905	133.904	135.905	137.905
Abundance (%)	0.11	0.10	2.42	7.85	71.70

*l.willmann@rug.nl

†s.knoop@vu.nl

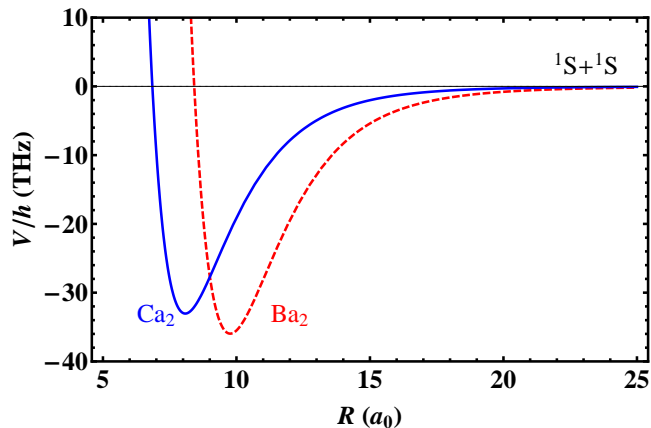


FIG. 1: (Color online) The $X^1\Sigma_g^+$ potentials of Ca_2 and Ba_2 as a function of internuclear distance. The solid blue curve is the potential of Ca_2 taken from Ref. [23]. The dashed red curve is the Tang-Toennies potential of Ba_2 taken from Ref. [24].

reduces the number of collision channels compared with the alkali metal systems.

To calculate the s -wave scattering length we solve the 1D radial Schrödinger equation with zero angular momentum and vanishing kinetic energy,

$$\psi''(R) + \frac{2\mu}{\hbar^2} [E - V(R)] \psi(R) = 0, \quad (1)$$

where μ is the reduced mass, R the internuclear distance, $V(R)$ the Born-Oppenheimer potential (here the $X^1\Sigma_g^+$ potential), and E the kinetic energy (below μK). The asymptotic form of the wavefunction is $\psi(R) \propto \sin[k(R - a)]$, where $k = \sqrt{2\mu E/\hbar^2}$, and a is the scattering length. We fit the asymptotic form to the solution of Eq. (1) for large R in order to obtain a . Within the Born-Oppenheimer approximation, the potentials are identical for all the isotopes of a particular atomic system. Therefore, for a given potential $V(R)$, one only needs to adjust μ to obtain a for all the isotopes.

To obtain reliable scattering lengths accurate potentials are needed. With the exception of systems with only a few electrons, like metastable helium [22], *ab initio* potentials are in general not accurate enough and constraints from experimental data are required. For Ca_2 an analytic representation of the $X^1\Sigma_g^+$ potential based on an extensive set of experimental data from the Tiemann group is available [23]. For Ba_2 such an accurate potential is not available. Here we rely on the analytical representation according to the Tang-Toennies potential model [24], which has shown to be able to reproduce accurately the $X^1\Sigma_g^+$ potentials of Ca_2 [25] and Sr_2 [24]. The used Ca_2 and Ba_2 potentials are shown in Fig. 1.

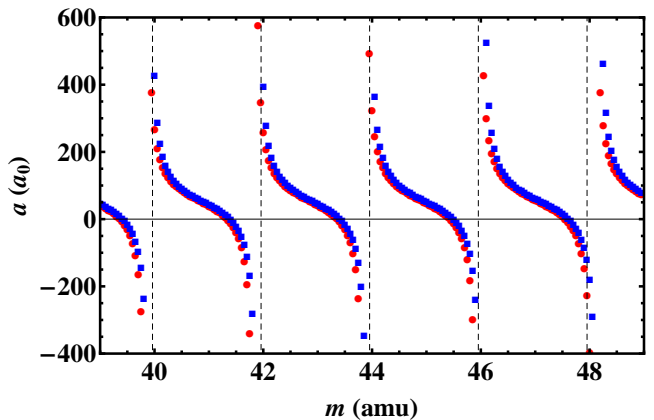


FIG. 2: (Color online) The mass dependence of the scattering length for Ca, using the $X^1\Sigma_g^+$ potential of Ref. [23], showing calculations with C_6 coefficients that give rise to $340a_0$ (red closed circles) and $700a_0$ (blue closed squares) for ^{40}Ca . The plotted mass is twice the reduced mass and the dashed vertical lines indicate the mass of the even isotopes of Ca.

III. RESULTS

A. Calcium

Information on the Ca_2 $X^1\Sigma_g^+$ potential has been gathered by several spectroscopic methods, including photoassociation spectroscopy [26–28], Fourier-transform spectroscopy [29] and filtered laser excitation technique [23]. Based on these detailed spectroscopic data, an interval of the scattering length for ^{40}Ca is determined to be $340 - 700a_0$ [28]. In the ^{40}Ca BEC experiment a scattering length of $a \approx 440a_0$ was estimated from a measurement of the chemical potential [6], without quoting an uncertainty. Therefore we take the scattering length range of $340 - 700a_0$ as starting point of our calculations.

We have taken the analytical representation and parameter values of the Ca_2 $X^1\Sigma_g^+$ potential from Ref. [23] (see Fig. 1). We allow the C_6 long-range coefficient to vary within a factor 0.991 to 1.003 from its reported value [23], in order to reproduce the scattering length interval for ^{40}Ca . We then take the mass as a variable parameter and calculate the scattering length for the full mass interval spanned by the stable even isotopes. In this way we transfer the knowledge on ^{40}Ca to the other isotopes.

The results for Ca are shown in Fig. 2. The plotted mass is twice the reduced mass, which for homonuclear collisions simply is the atomic mass. The dashed vertical lines indicate the masses of the even isotopes, from which the scattering lengths for homonuclear collisions are directly read off. Two calculations are shown, obtained from potentials with C_6 coefficients that give rise to $340a_0$ (red closed circles) and $700a_0$ (blue closed squares) for ^{40}Ca . The scattering length shows the expected behavior as a function of mass, with a regular pattern of scattering resonances. They can be understood from the mass

TABLE II: Scattering lengths of even Ca isotopes (left), as well as interisotopic scattering lengths for all combinations with ^{40}Ca , and $^{42}\text{Ca}+^{44}\text{Ca}$ (right).

	$a \text{ (} a_0 \text{)}$		$a \text{ (} a_0 \text{)}$
40+40	+340 ... + 700 [28]	40+42	+45 ... + 50
42+42	+320 ... + 640	40+44	$\pm\infty$
44+44	+460 ... + 1800	40+46	+62 ... + 68
46+46	$\pm\infty$	40+48	-66 ... - 39
48+48	-230 ... -120	42+44	+47 ... + 52

dependence of the vibrational splitting, and therefore the number of bound states. A scattering resonance appears at those mass values at which a new vibrational state becomes bound, i. e. where the least bound vibrational state has zero binding energy. We find that accidentally all even isotopes are located close to such a scattering resonance, giving rise to large positive or negative scattering lengths.

The scattering length intervals for the different isotopes are given in Table II. It is clear that Ca does not provide an isotope with a favorable scattering length. At most one can state that ^{42}Ca has a slightly smaller scattering length than ^{40}Ca . In addition, the interisotope scattering lengths are given for collisions between ^{40}Ca and the other isotopes, and $^{42}\text{Ca}+^{44}\text{Ca}$. Here we find favorable scattering lengths for $^{40}\text{Ca}+^{42}\text{Ca}$, $^{40}\text{Ca}+^{46}\text{Ca}$ and $^{42}\text{Ca}+^{44}\text{Ca}$. Taking into consideration the large scattering length of ^{44}Ca and ^{46}Ca , the only interesting mixture in view of sympathetic cooling is $^{40}\text{Ca}+^{42}\text{Ca}$.

B. Barium

Knowledge of the $\text{Ba}_2 X^1\Sigma_g^+$ potential is sparse, because of a limited amount of experimental data [30, 31], which cover only a small part of the vibrational spectrum. Similarly, theoretical data is scarce. The binding energies of Ba_2 were calculated by Jones [32]. First wave function based quantum chemical calculation was reported by Ref. [33], most recently by Ref. [34]. The most accurate calculations of the long-range coefficients C_6 , C_8 , C_{10} are reported by Porsev and Derevianko [35, 36].

We have used the Tang-Toennies potential [37] of Ref. [24] to model the $\text{Ba}_2 X^1\Sigma_g^+$ potential as

$$V(R) = Ae^{-bR} - \sum_{n=3}^5 \left(1 - e^{-bR} \sum_{k=0}^{2n} \frac{(bR)^k}{k!} \right) \frac{C_{2n}}{R^{2n}}, \quad (2)$$

where the short-range parameters (in a.u.) $A = 105.4$ and $b = 0.9657$ are obtained from rescaling an accurate $\text{Sr}_2 X^1\Sigma_g^+$ potential [38], using the measured fundamental vibration frequency [31], and taking the long-range coefficients from Ref. [35, 36] (see Fig. 1).

Although we do not expect the potential to be accurate enough to predict the scattering length, we can use it to investigate its mass dependence. The result is shown in

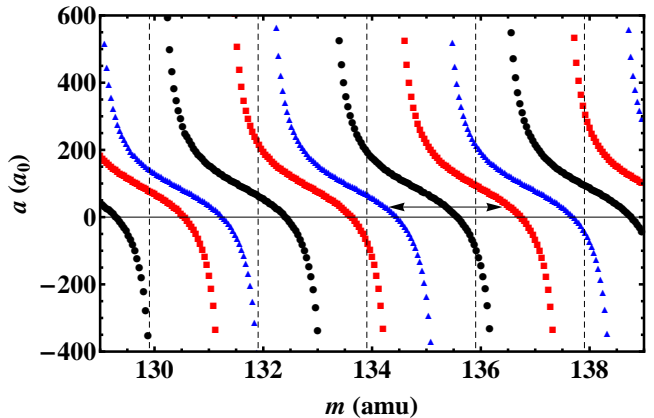


FIG. 3: (Color online) The mass dependence of the scattering length for Ba, using the Tang-Toennies model to represent the $X^1\Sigma_g^+$ potential with the parameter values from Ref. [24] (black closed circles). The arrow indicates the effect of the uncertainty in the theoretical C_6 coefficient, showing its lower (blue closed triangles) and upper (red closed squares) limit. The plotted mass is twice the reduced mass and the dashed vertical lines indicate the mass of the even isotopes of Ba.

Fig. 3 (black closed circles). We observe that the spacing between the resonances is larger than that between the even isotopes, giving rise to a variety of scattering lengths among the different isotopes. Therefore it is very probable that at least one of the isotopes has a favorable scattering length for BEC formation.

In addition, we have investigated the effect of the theoretical uncertainty in the reported C_6 coefficient, 5160 ± 74 a. u. [35, 36]. We have repeated the above calculation with the upper (red closed squares) and lower (blue closed triangles) limits (see Fig. 3). Note that these adjustments in C_6 also require small changes in A and b [24]. The uncertainty in C_6 gives rise to a large spread in the scattering length, which can also be seen as a large shift along the mass axis, as indicated by the arrow. This means that even if an accurate short-range potential would be available, still no precise prediction of the scattering length is possible. On the other hand, whereas the scattering length itself is extremely sensitive to details of the potential, the spacing between the scattering resonances is not. Therefore, once scattering length information of one of the isotopes becomes available, the simple Tang-Toennies potential is sufficient to predict the scattering lengths of all the other isotopes [40], at least at an accuracy that allows to choose the best isotope to achieve BEC.

IV. CONCLUSION AND OUTLOOK

In summary, we have investigated the s -wave scattering lengths of the Ca and Ba even (bosonic) isotopes. An experimentally accurate ground state potential of Ca_2

enabled us to calculate the scattering lengths for all the isotopes, taking knowledge of ^{40}Ca scattering length as a reference. We have observed that accidentally scattering resonances appear near all even isotopes, leading to large positive and negative scattering lengths for all isotopes. Only ^{42}Ca shows a small improvement in terms of scattering length compared to ^{40}Ca . Therefore, alternative methods to that of evaporative cooling are interesting for Ca, such as direct laser cooling into quantum degeneracy using a narrow transition [39].

In addition, scattering lengths for all the even Ba isotopes have been investigated using a Tang-Toennies model potential. In contrast to the Ca case, here the scattering lengths vary strongly over the isotopes, resulting in a high probability that at least one isotope has a favorable scattering length to produce a BEC. More accurate knowledge of the ground state Ba_2 potential, including the long-range coefficients, based on experimental data that covers the full vibrational spectrum is

needed for an improved determination of the scattering lengths. However, once experimental knowledge on the scattering length of one isotope becomes available, the scattering lengths of all the other isotopes can be predicted with the present model potential.

Acknowledgments

We thank Erling Riis and Wim Vassen for careful reading of the manuscript and useful comments. This work has been performed as part of the research program of the *Stichting voor Fundamenteel Onderzoek der Materie* (FOM) through programme 114 (TRI μ P), which is financially supported by the *Nederlandse Organisatie voor Wetenschappelijk Onderzoek* (NWO). S. K. acknowledges financial support from NWO (VIDI grant).

-
- [1] K. Burnett, P. S. Julienne, P. D. Lett, E. Tiesinga, and C. J. Williams, *Nature* **416**, 225 (2002).
 - [2] A. D. Ludlow *et al.*, *Science* **319**, 1805 (2008).
 - [3] N. D. Lemke *et al.*, *Phys. Rev. Lett.* **103**, 063001 (2009).
 - [4] A. Derevianko and H. Katori, *Rev. Mod. Phys.* **83**, 331 (2011).
 - [5] A. J. Daley, M. M. Boyd, J. Ye, and P. Zoller, *Phys. Rev. Lett.* **101**, 170504 (2008).
 - [6] S. Kraft, F. Vogt, O. Appel, F. Riehle, and U. Sterr, *Phys. Rev. Lett.* **103**, 130401 (2009).
 - [7] S. Stellmer, M. K. Tey, B. Huang, R. Grimm, and F. Schreck, *Phys. Rev. Lett.* **103**, 200401 (2009).
 - [8] Y. N. Martinez de Escobar *et al.*, *Phys. Rev. Lett.* **103**, 200402 (2009).
 - [9] S. Stellmer, M. K. Tey, R. Grimm, and F. Schreck, *Phys. Rev. A* **82**, 041602(R) (2010).
 - [10] P. G. Mickelson, Y. N. Martinez de Escobar, M. Yan, B. J. DeSalvo, and T. C. Killian, *Phys. Rev. A* **81**, 051601(R) (2010).
 - [11] Y. Takasu *et al.*, *Phys. Rev. Lett.* **91**, 040404 (2003).
 - [12] T. Fukuhara, S. Sugawa, and Y. Takahashi, *Phys. Rev. A* **76**, 051604(R) (2007).
 - [13] T. Fukuhara, S. Sugawa, Y. Takasu, and Y. Takahashi, *Phys. Rev. A* **79**, 021601(R) (2009).
 - [14] S. Sugawa, R. Yamazaki, S. Taie, and Y. Takahashi, *Phys. Rev. A* **84**, 011610(R) (2011).
 - [15] A. Stein, H. Knöckel, and E. Tiemann, *Eur. Phys. J. D* **57**, 171 (2010).
 - [16] T. Zelevinsky, *Physics* **2**, 94 (2009).
 - [17] S. Hoekstra, A. K. Mollema, R. Morgenstern, H. W. Wilschut, and R. Hoekstra, *Phys. Rev. A* **71**, 023409 (2005).
 - [18] U. Dammalapati, I. Norris, C. Burrows, A. S. Arnold, and E. Riis, *Phys. Rev. A* **81**, 023424 (2010).
 - [19] S. De, U. Dammalapati, K. Jungmann, and L. Willmann, *Phys. Rev. A* **79**, 041402(R) (2009).
 - [20] Y. Geng-Hua, Z. Jia-Qi, L. Rung-Bing, W. Jin, and Z. Ming-Sheng, *Chin. Phys. Lett.* **28**, 073201 (2011).
 - [21] J. E. Sansonetti and W. C. Martin, *J. Phys. Chem. Ref. Data* **34**, 1559 (2005).
 - [22] M. Przybytek and B. Jeziorski, *J. Chem. Phys.* **123**, 134315 (2005).
 - [23] O. Allard, C. Samuelis, A. Pashov, H. Knöckel, and E. Tiemann, *Eur. Phys. J. D* **26**, 155 (2003).
 - [24] P. Li, J. Ren, N. Niu, and K. T. Tang, *J. Phys. Chem. A* **115**, 6927 (2011).
 - [25] D. D. Yang, P. Li, and K. T. Tang, *J. Phys. Chem.* **131**, 154301 (2009).
 - [26] G. Zinner, T. Binnewies, F. Riehle, and E. Tiemann, *Phys. Rev. Lett.* **85**, 2292 (2000).
 - [27] C. Degenhardt *et al.*, *Phys. Rev. A* **67**, 043408 (2003).
 - [28] F. Vogt *et al.*, *Eur. Phys. J. D* **44**, 73 (2007).
 - [29] O. Allard, A. Pashov, H. Knöckel, and E. Tiemann, *Phys. Rev. A* **66**, 042503 (2002).
 - [30] R. M. Clements and R. F. Barrow, *J. Chem. Soc. Faraday Trans. 2* **81**, 625 (1985).
 - [31] M. A. Lebeault, J. Viallon, V. Boutou, and J. Chevalerey, *J. Mol. Spectrosc.* **192**, 179 (1998).
 - [32] R. O. Jones, *J. Chem. Phys.* **71**, 1300 (1979).
 - [33] A. Allouche, M. Aubert-Frecon, G. Nicolas, and F. Spiegelmann, *Chem. Phys.* **200**, 63 (1995).
 - [34] A. V. Mitin, *Rus. J. Phys. Chem.* **83**, 1160 (2009).
 - [35] S. G. Porsev and A. Derevianko, *Phys. Rev. A* **65**, 020701(R) (2002).
 - [36] S. G. Porsev and A. Derevianko, *J. Exp. Theor. Phys.* **102**, 195 (2006).
 - [37] K. T. Tang and J. P. Toennies, *J. Chem. Phys.* **80**, 3726 (1984).
 - [38] A. Stein, H. Knöckel, and E. Tiemann, *Phys. Rev. A* **78**, 042508 (2008).
 - [39] C. S. Adams, S. G. Cox, E. Riis, and A. S. Arnold, *J. Phys. B: At. Mol. Opt. Phys.* **36**, 1933 (2003).
 - [40] We have applied the Tang-Toennies potential model for Ca_2 [25] and Sr_2 [24], from which we have obtained similar results as in Sec. III A and Ref. [15], respectively, when finetuning the C_6 coefficient to reproduce the scattering length of one particular isotope.